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ELECTRON IMPACT RATE COEFFICIENTS FOR THE LOW LYING METASTABLE --ETC(U)
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NRL Memorandum Report 3371

Electron Impact Rate Coefficients for the Low Lying Metastable States of O, O^+, N and N^+

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Plasma Physics Divison

September 1976

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A set of electron impact excitation rate coefficients for the low lying metastable states of O, N, O^+, and N^+ are presented. These rates are obtained using recent and more accurate cross sections. These species play an important role in the emission, deionization processes and communication problems of a disturbed atmosphere.

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N(+)

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Low Lying Metastable States of O, O^+, N and N^+

INTRODUCTION

The atmosphere, from the sea level to the F-region of the ionosphere can be ionized by many external forces. These disturbing forces include, the lightning discharges, the passage of charged particle beams, the passage of laser beams, the solar flares, the cosmic rays and the atmospheric nuclear bursts. The ionization of the atmosphere under these external forces results in the creation of a large number of excited atomic and molecular species and their corresponding ions which also are in excited states. In addition, the free electrons ejected under the ionization force possess enough kinetic energy to alter the distribution of these species.

Among the atomic and atomic ions species of the disturbed atmosphere, the following excited metastable states play an important role in the chemistry of the atmosphere. These are: $O(^1D)$, $O(^1S)$, $O^+(^2D)$, $O^+(^2P)$, $N(^2D)$, $N(^2P)$, $N^+(^1D)$ and $N^+(^1S)$. These metastable states lie close, within few eV, to the ground state of their respective species. Their densities are controlled to a large degree by electron excitation and de-excitation processes in addition to recombination, charge exchange, and ion-molecule rearrangements (for the ionic species only).

In order to calculate the deionization process of such a disturbed atmosphere, its emission, the conductivity of a disturbed channel and other parameters, one must know the electron temperature and a wide range of inelastic collision cross sections. The collision cross sections of electrons with the species mentioned above, and the relevant rate coefficients, are essential for calculations of relevant parameters.

The rate coefficients and the collision strengths for the inelastic processes of the free electrons with these species have been reported.[1,2]

Note: Manuscript submitted September 3, 1976.

However, due to the availability of better cross sections we present a new set of rate coefficients for excitations among these low lying metastable states.

NITROGEN ATOM LOW LYING METASTABLE STATES

The low lying metastable states of nitrogen are $N(^2D)$ and $N(^2P)$. The rate coefficients for the electron impact excitations of $N(^4S)$ - $N(^2D)$, $N(^4S)$ - $N(^2P)$ and $N(^2D)$ - $N(^2P)$, reported earlier[1] were based on cross sections calculated by Henry et al.[3] These calculations, however, neglected the polarization of the target atom during the collision, incomplete allowance for short range correlations and omissions of higher lying configurations. A recent electron-nitrogen atom scattering calculations by Berrington, et al[4] includes all these effects. We have elected these cross sections to obtain the relevant rates. Figures 1-3 show these cross sections and are compared with those of Henry et al.[3] and Ormonde, et al.[5]

We have utilized these current cross sections[4] to obtain, in the usual manner,[6] the relevant electron impact excitation rate coefficients. These rates are given numerically in Table 1 and are shown graphically in Fig. 4. Comparison of these rates with the rates reported previously[1] show that the current rates are significantly smaller for $N(^4S)$ - $N(^2D)$ at low T_e. This is due obviously to the difference in the cross sections (see Fig. 1). It should be also stated that, the resonance structure in the cross section $N(^2D)$ - $N(^2P)$ (see Fig. 3), was ignored in obtaining the current relevant corresponding rate.

OXYGEN ATOM LOW LYING METASTABLE STATES

The low lying metastable states of oxygen are $O(^1D)$ and $O(^1S)$. The rate coefficients for the electron impact excitations of $O(^3P)$ - $O(^1D)$, $O(^3P)$ - $O(^1S)$ and $O(^1D)$ - $O(^1S)$ reported earlier[1] were based on the cross sections calculated by Henry, et al.[3] However, the current relevant rate coefficients reported in this section are based on the recent, more accurate, cross sections calculated by Thomas and Nisbet.[7] These cross sections are shown in Fig. 5 along with Henry et al.[3] and Vo Ky Lan et al.[8] It is obvious from this figure that there is very little change

in the cross section for $O(^3P) - O(^1S)$, therefore we shall retain the rate calculated earlier.[1] However, the changes are obvious near threshold and above for $O(^3P) - O(^1D)$, and above threshold for $O(^1D) - O(^1S)$. The new rate coefficients for the low lying oxygen metastable states are given in Table 2 and are shown in Fig. 6.

THE COLLISION STRENGTHS FOR THE LOW LYING METASTABLE STATES OF N^+ AND O^+

The metastable, low lying, excited states of N^+ are $N^+(^1D)$ and $N^+(^1S)$. Those for O^+ are $O^+(^2D)$ and $O^+(^2P)$. The collision strength for most of these states in O^+ and N^+ have been calculated by Henry, et al.[3] and more recently for O^+ by Czyzak, et al.[9] For oxygen ion, the results of Refs. (3) and (9) are in close agreement (within 10%). As for N^+, Henry et al.[3] results are in good agreement with those calculated by Saraph, et al.[10] Therefore, for calculational purposes one may select the collision strengths, for O^+ and N^+, as given by Henry et al.[3] These values are given in Table 3.

In electron ion collision, the cross section is finite at threshold and so is the collision strength. This latter varies slowly as a function of incident electron energy over ranges of interest. Therefore, one can utilize these collision strengths to obtain the relevant electron impact excitation or de-excitation rate coefficients.

The de-excitation rate coefficient from level j to i (j > i) is[11]

$$Y_{ji} = \frac{8.63 \times 10^{-6} \, \gamma(i, j)}{g_j \sqrt{T}} \qquad (1)$$

with g_j being the statistical weight of level j and

$$\gamma(j, i) = \int_0^\infty \Omega(j, i) \, \mathrm{Exp}\left(\frac{E}{kT}\right) d\left(\frac{E}{kT}\right) \qquad (2)$$

In Eq. (2) E is the electron energy, T is the electron temperature in $^\circ K$ and $\Omega(j, i)$ is the collision strength. Equation (2) represents the

averaging of the cross section and the electron velocity over a Maxwellian velocity distribution. When the collision strength is constant i.e. it does not depend on E then Eq. (1) is used to obtain the de-excitation rate coefficient. The excitation rate coefficient can be obtained via the detailed balancing.

Using the collision strengths given in Table 3 and Eq. (1), the corresponding de-excitation rate coefficients are given in Table 4.

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TABLE 1

Electron Impact Excitation Rate Coefficients for the Low Lying States of Nitrogen Atom

T_e(eV)	^4S - ^2D	^4S - ^2P	^2D - ^2P
0.1	8.0 (- 20)	2.6 (- 25)	2.10 (- 14)(*)
0.2	1.54 (- 14)	2.03 (- 17)	1.16 (- 11)
0.3	1.25 (- 12)	1.11 (- 14)	9.78 (- 11)
0.5	4.2 (- 11)	1.47 (- 12)	6.0 (- 10)
0.7	1.98 (- 10)	1.63 (- 11)	1.16 (- 9)
1.0	6.38 (- 10)	8.91 (-11)	2.05 (- 9)
1.2	1.08 (- 9)	1.73 (- 10)	2.56 (- 9)
1.5	1.52 (- 9)	3.38 (- 10)	3.24 (- 9)
2.0	2.27 (- 9)	6.54 (- 10)	4.1 (- 9)
3.0	3.31 (- 9)	1.23 (- 9)	5.18 (- 9)
5.0	4.50 (- 9)	1.99 (- 9)	6.2 (- 9)
7.0	5.26 (- 9)	2.36 (- 9)	6.5 (- 9)
10.0	5.85 (- 9)	2.4 (- 9)	6.5 (- 9)
15.0	5.97 (- 9)	2.49 (- 9)	6.1 (- 9)
20.0	4.96 (- 9)	2.28 (- 9)	5.47 (- 9)

(*) Numbers in parenthesis indicate the power of ten by which the entries are multiplied.

TABLE 2

Electron Impact Excitation Rate Coefficients for the Low Lying States of Oxygen Atom

T_e(eV)	^3P - ^1D	^3P - ^1S	^1D - ^1S
0.1	1.92 (- 18)	1.78 (- 28)	2.25 (- 19)(*)
0.2	5.28 (- 14)	1.96 (- 19)	1.76 (- 14)
0.3	1.76 (- 12)	2.10 (- 16)	8.07 (- 13)
0.5	3.28 (- 11)	6.04 (- 14)	1.52 (- 11)
0.7	1.21 (- 10)	7.25 (- 13)	5.4 (- 11)
1.0	3.43 (- 10)	4.93 (- 12)	1.38 (- 10)
1.2	5.20 (- 10)	1.06 (- 11)	1.97 (- 10)
1.5	7.94 (- 10)	2.32 (- 11)	2.76 (- 10)
2.0	1.21 (- 9)	5.15 (- 11)	3.98 (- 10)
3.0	1.84 (- 9)	1.16 (- 10)	5.30 (- 10)
5.0	2.52 (- 9)	2.21 (- 10)	7.16 (- 10)
7.0	2.73 (- 9)	2.8 (- 10)	7.76 (- 10)
10.0	2.80 (- 9)	3.3 (- 10)	7.5 (- 10)
15.0	2.58 (- 9)	3.8 (- 10)	6.9 (- 10)
20.0	2.23 (- 9)	3.7 (- 10)	6.4 (- 10)

(*) Numbers in parenthesis indicate the power of ten by which the entries are multiplied.

TABLE 3

Collision Strengths for the Electron Impact Excitations of the Low Lying Metastable States of O^+

Transition	Collision Strength
$O^+(^4S) - O^+(^2D)$	1.57
$O^+(^4S) - O^+(^2P)$	0.475
$O^+(^2D) - O^+(^2P)$	1.77
$N^+(^3P) - N^+(^1D)$	2.98
$N^+(^3P) - N^+(^1S)$	0.395
$N^+(^1D) - N^+(^1S)$	0.41

TABLE 4

De-excitation Rate Coefficients for the Low Lying Metastable States of O^+ and N^+. T_e is in units of eV.

Transition	g_j	De-excitation Rate Coefficient
$^2D - {}^4S$	10	$\frac{1.26 \times 10^{-8}}{\sqrt{T_e}}$
$^2P - {}^4S$	6	$\frac{6.33 \times 10^{-9}}{\sqrt{T_e}}$
$^2P - {}^2D$	6	$\frac{2.36 \times 10^{-8}}{\sqrt{T_e}}$
$^1D - {}^3P$	5	$\frac{4.77 \times 10^{-8}}{\sqrt{T_e}}$
$^1S - {}^3P$	1	$\frac{3.16 \times 10^{-8}}{\sqrt{T_e}}$
$^1S - {}^1D$	1	$\frac{3.28 \times 10^{-8}}{\sqrt{T_e}}$

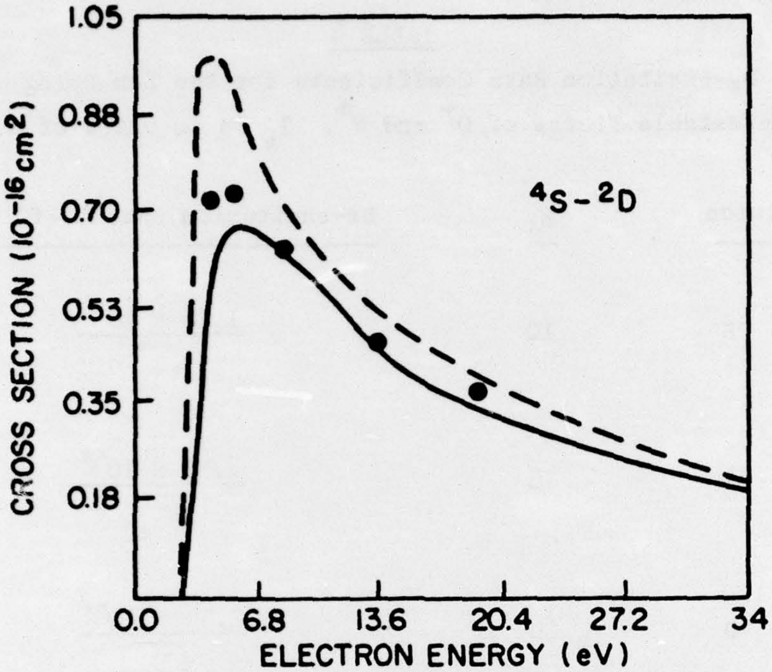

Fig. 1 — *Electron impact excitation cross section for* N(^{4}S) — N(^{2}D). Solid curve Ref. (4), dashed curve Ref. (3), and circles Ref. (5).

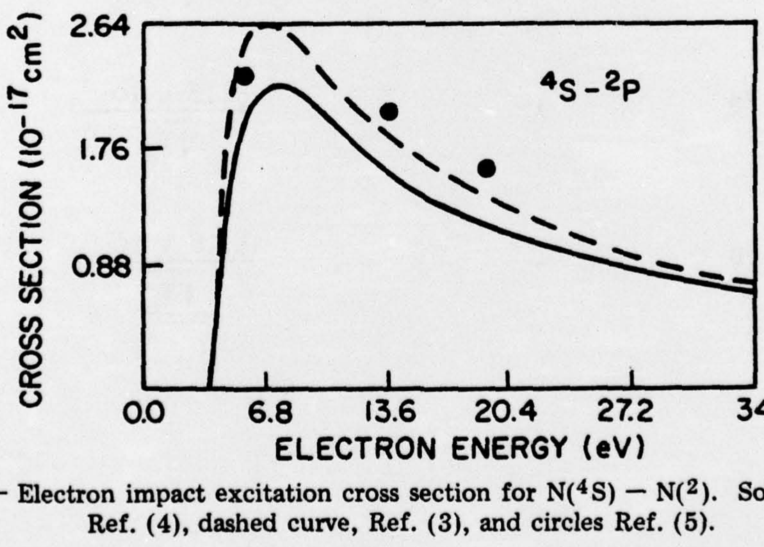

Fig. 2 — Electron impact excitation cross section for N(^{4}S) — N(^{2}). Solid curve Ref. (4), dashed curve, Ref. (3), and circles Ref. (5).

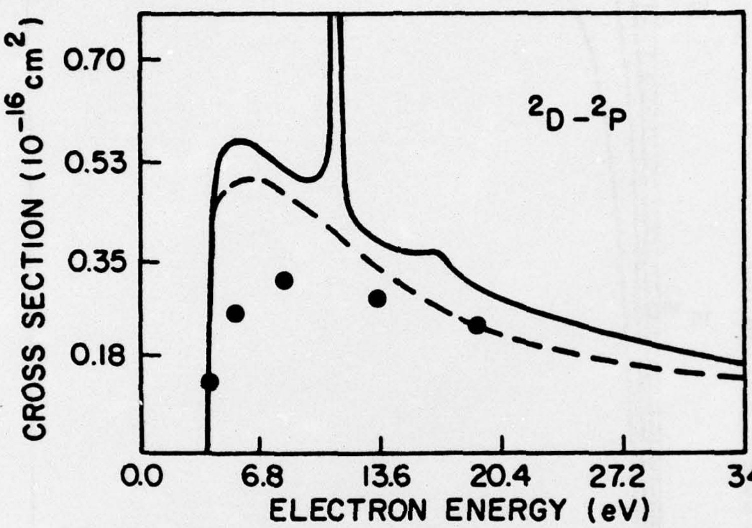

Fig. 3 — Electron impact excitation cross section for N(^{2}D) — N(^{2}). Solid curve Ref. (4), dashed curve Ref. (3) and circles Ref. (5).

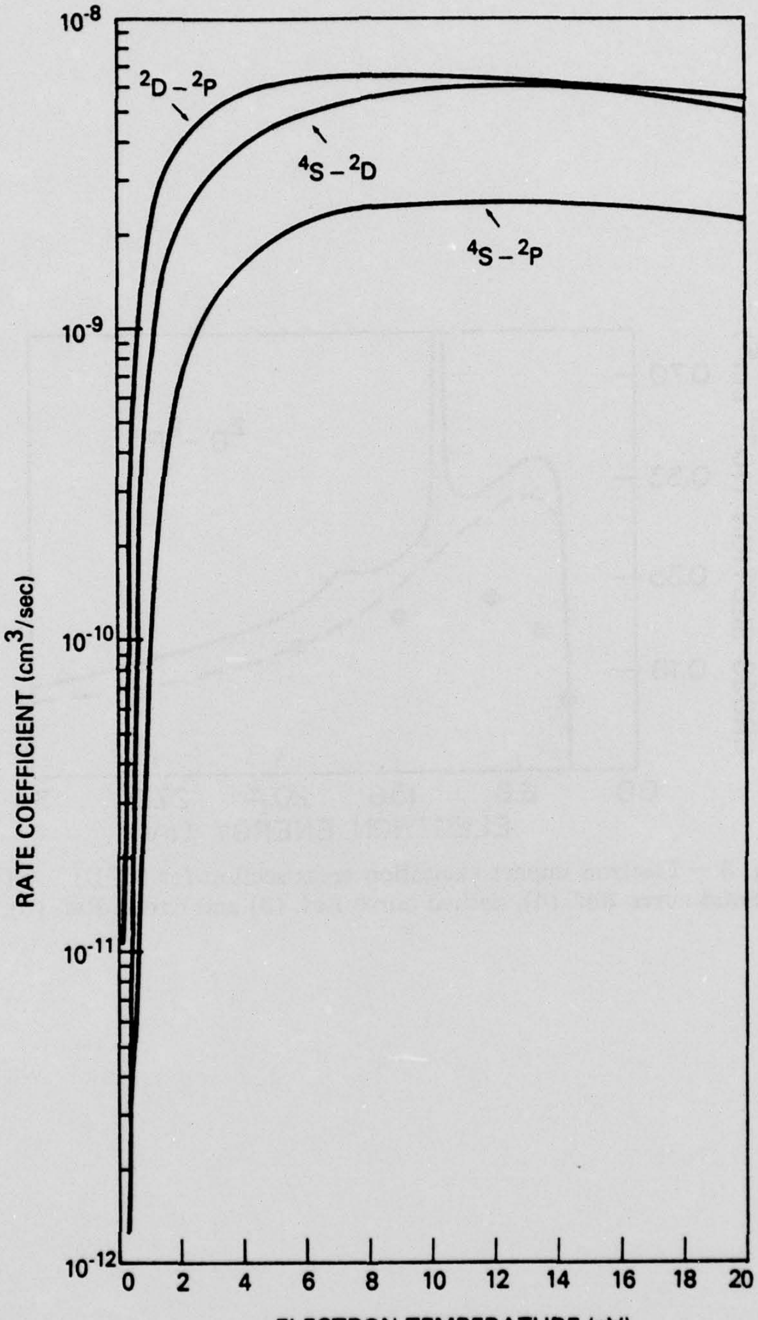

Fig. 4 — Excitation rate coefficients for the low lying metastable states of nitrogen atom as a function of the electron temperature

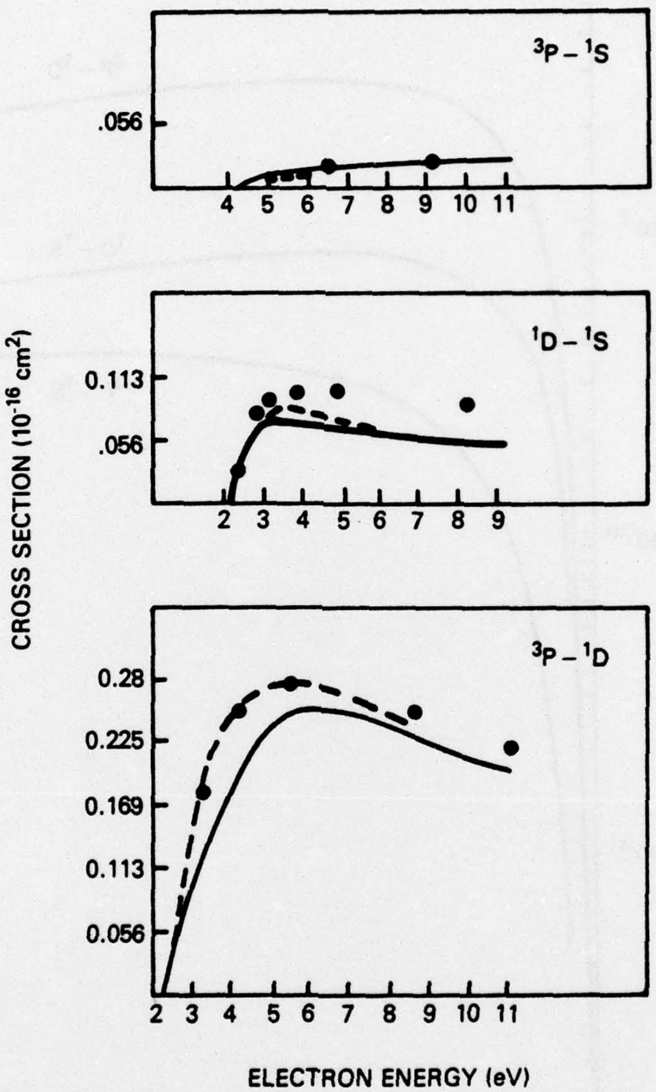

Fig. 5 — Electron impact excitation cross sections for low lying metastable states of oxygen. Solid curve Ref. (7), dashed curve Ref. (8), and circles Ref. (3).

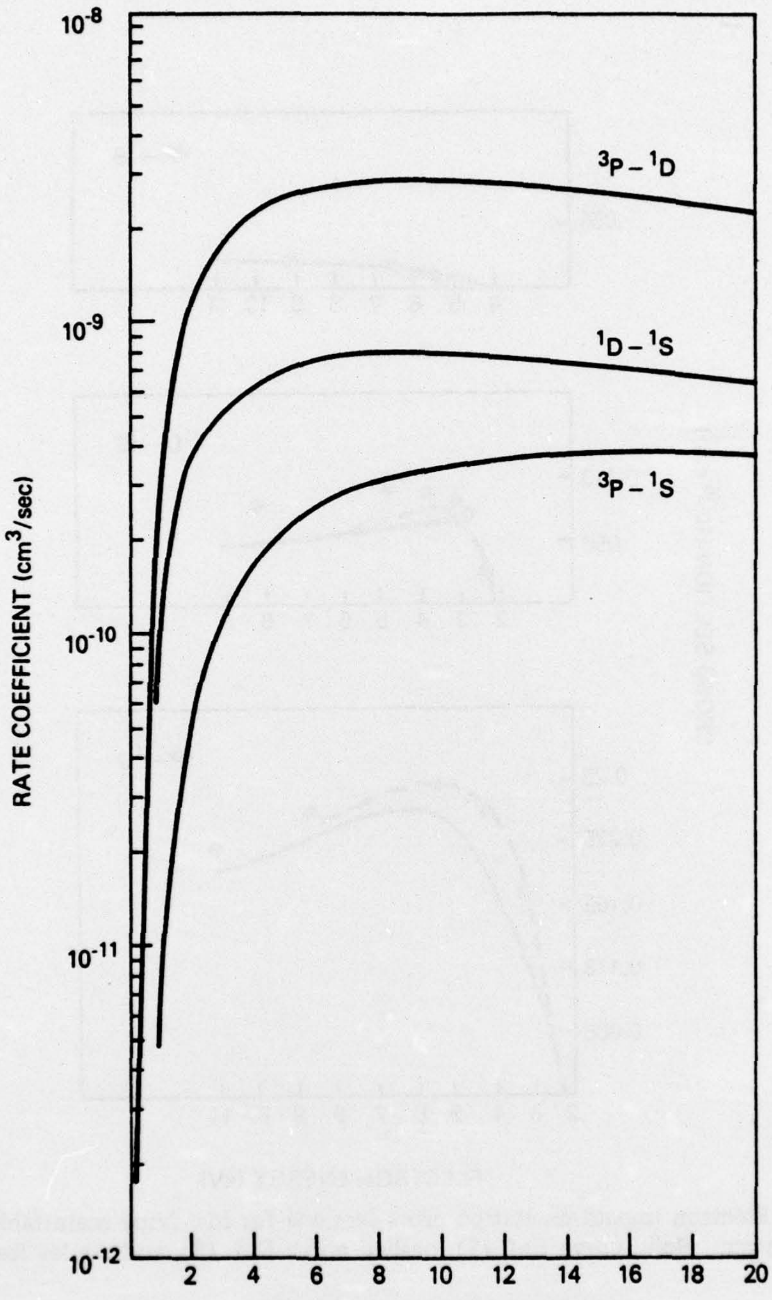

Fig. 6 — Electron impact excitation rate coefficient for $O(^3P) - O(^1D)$, $O(^3P) - O^1S)$ and $O(^1D) - O(^1S)$ as a function of the electron temperature

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